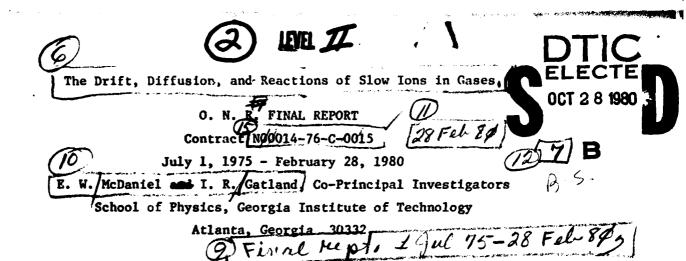


MICROCOPY RESOLUTION TEST CHART



1. Scientific Problem

The experimental program consisted of measurements of the mobilities and longitudinal diffusion coefficients of ions in various gases at room temperature. By varying the energy parameter (E/N) of the ions, we may vary the average ionic energy from the thermal value at 300°K to about 10 eV. Our measured mobilities and diffusion coefficients are useful in calculations of properties of weakly ionized plasmas. In addition, the mobilities as a function of E/N can be inverted to obtain the interaction potential for the ion-neutral combination involved, and the mobilities are also useful in calculations of the rate of positive ion-negative ion recombination. Rate coefficients measured for ion-molecule reactions play a role in explaining plasma chemistry; ionic transport data are required for the accurate determination of these rate coefficients. Observations on ionic identity and abundances as functions of gas pressure and temperature are particularly important in atmospheric research.

The relevance of ionic transport phenomena to atmospheric problems arises partly from the concomitant transport of charge, mass, momentum, and energy through space. Further, the drift of ions in an electric field can significantly increase the kinetic energy of the ions, and can change their internal excitation energy by ion-molecule collisions. The changes in translational and internal energy can markedly affect the rates of ion-molecule reactions, and subsequently the rates of other kinds of collisions, notably ion-ion and electron-ion recombination, in the atmosphere.

The theoretical program consisted of the calculation of mobilities and diffusion coefficients from given potentials for several particularly interesting ion-neutral systems, the determination of interaction potentials from mobility data using the standard two-temperature theory, investigation of the three-temperature theory in relation to diffusion, and initial studies of polyatomic cases.

Approved for public release;
Distribution Unlimited

P

From our standpoint the most important use of the mobility data is to generate ion-neutral interaction potentials covering a very wide range of ion-neutral separation distance by inverting the experimental data. The interaction potential for a two-particle system is one of the most fundamental properties of the system. It determines the mutual scattering behavior of the particles and hence the transport properties. The interaction potential also determines many properties of the system that is formed if the two particles can temporarily or permanently combine. In the case of radiative processes, for example, the interaction potentials for the upper and ground states of a neutral diatomic molecule or ion are required for the determination of the wave functions, transition probabilities and spectral features. The standard beam scattering technique used to obtain information about the interaction potential for an ion-neutral system covers a much smaller range of separation distance than does the new method described here. The interaction potentials obtained for the halogen ion-rare gas combinations may have applications in excimer lasers.

We also calculate from our measured drift velocities the zero-field mobilities of these ions in various gases at temperatures ranging from  $300^{\circ}$ K to  $\sim 10^4$   $^{\circ}$ K by the techniques we have described in Ref. 2 of Section 3.

## 2. Scientific and Technical Approach

The experiments are performed with a drift tube mass spectrometer, by techniques which permit accurate measurements to be made on individual ionic species even though several species may be simultaneously present and coupled by ion-molecule reactions. The drift tube gas is maintained at room temperature, but the average energy of a given species of ion can be varied from very close to thermal energy up to a maximum of about 10 eV in favorable cases. The average energy of the ions of a given type is determined by the parameter E/N, where E is the intensity of the electrostatic drift field and N is the number density of the neutral gas molecules contained in the drift tube. The measurements are made as a function of E/N.

The basic measurement made is of the arrival time spectra for each separate ionic species in the drift tube. The measurements are made as functions of drift distance, electric field strength (E) in the drift region, number density of gas molecules in the drift tube (N), and the energy parameter (E/N).

The theoretical calculations are concerned with the relation between the ion-neutral interaction potential and the measured values of the mobilities and diffusion coefficients. The calculation of the transport coefficients is based on a moment solution of the appropriate Boltzmann equation with basis functions which reflect the sometimes high random energy derived from the electric field and the non-symmetric character of the ionic velocity. This allows the mobility data to be used to test theoretical potentials and also to serve as an integral part of an iteration technique which determines the interaction potential directly from the data.

## 3. Results and Publications

The results that we obtained during the period covered by this report are indicated by the titles in the list of publications that follows. Also given in this list are the names of all of the scientific personnel who participated in the research. Of these personnel, the following have obtained their Ph.D. degrees in Physics at the Georgia Institute of Technology: W. F. Morrison (1975), D. R. James (1975), and G. R. Akridge (1976). M. G. Thackston will obtain his Ph.D. degree in December 1980, and D. R. Lamm in 1981.

Acces	sion For		
NTIS	GRA&I	A	
DTIC	TAB		
Unannounced 🔲			
Justi	fication_		
Ву			
Distr	ibution/		
Avai	lability	Codes	
	Avail and	/or	
Dist	Special	1	
	1 1	•	
A			

## **PUBLICATIONS**

- W. F. Morrison, G. R. Akridge, H. W. Ellis, R. Y. Pai, E. W. McDaniel, L. A. Viehland, and E. A. Mason, "Test of the Li<sup>+</sup> - He Interaction Potential", Jour. Chem. Phys. 63, 2238 (1975).
- 2. E. A. Mason, L. A. Viehland, H. W. Ellis, D. R. James, and E. W. McDaniel, "The Mobilities of K+ Ions in Hot Gases", Phys. Fluids 18, 1070 (1975).
- 3. R. Y. Pai, H. W. Ellis, G. R. Akridge, and E. W. McDaniel, "Longitudinal Diffusion Coefficients of Li<sup>+</sup> and Na<sup>+</sup> Ions in He, Ne, and Ar: Experimental Test of the Generalized Einstein Relation", J. Chem. Phys. 63, 2916 (1975).
- 4. R. Y. Pai, H. W. Ellis, G. R. Akridge, and E. W. McDaniel, "Generalized Einstein Relation: Application to Ions in Molecular Gases", Phys. Rev. A 12, 1781 (1975).
- 5. H. W. Ellis, R. Y. Pai, and E. W. McDaniel, "Mobilities of Li<sup>+</sup> and Na<sup>+</sup> Ions in Hydrogen Gas", J. Chem. Phys. <u>64</u>, 3492 (1976).
- 6. R. Y. Pai, H. W. Ellis, and E. W. McDaniel, "The Generalized Einstein Relation Application to Li<sup>+</sup> and Na<sup>+</sup> Ions in Hydrogen Gas", J. Chem. Phys. 64, 4238 (1976).
- 7. M. G. Thackston, H. W. Ellis, R. Y. Pai, and E. W. McDaniel, "Mobilities of Rb<sup>+</sup> Ions in He, Ne, Ar, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, and CO<sub>2</sub>", J. Chem. Phys. 65, 2037 (1976).
- 8. H. W. Ellis, M. G. Thackston, R. Y. Pai, and E. W. McDaniel, "Longitudinal Diffusion Coefficients of Rb<sup>+</sup> Ions in He, Ne, Ar, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, and CO<sub>2</sub>", J. Chem. Phys. 65, 3390 (1976).
- 9. H. W. Ellis, R. Y. Pai, E. W. McDaniel, E. A. Mason, and L. A. Viehland, "Transport Properties of Gaseous Ions Over a Wide Energy Range", Atomic Data and Nuclear Data Tables 17, 177-210 (1976).
- 10. I. R. Gatland, "Ion-Neutral Interaction Potentials and Gaseous Ion Diffusion Coefficients from Mobility Data", Fourth Int. Conf. on Atomic Physics, Berkeley, Calif., July 1976.
- 11. E. W. McDaniel, invited paper, "Studies of Ion Plasma Chemistry with Drift Tube Mass Spectrometers", Third International Symposium on Plasma Chemistry, Limoges, France, (July 1977).
- 12. E. W. McDaniel, invited paper, "Gaseous Ion Transport and Reaction Studies Using Drift Tube Mass Spectrometers", Presented at the U.S.-Japan Joint Seminar on the Glow Discharge and Its Fundamental Processes, Boulder, Colorado, (July 12-15, 1977).
- I. R. Gatland, W. F. Morrison, H. W. Ellis, M. G. Thackston, E. W. McDaniel, M. H. Alexander, L. A. Viehland, and E. A. Mason, "The Li<sup>+</sup> He Interaction Potential", Jour. Chem. Phys. 66, 5121 (1977).

- 14. I. R. Gatland, E. W. McDaniel, H. W. Ellis, M. G. Thackston, F. L. Eisele, and W. M. Pope, "Cs<sup>+</sup> Kr and Cs<sup>+</sup> Xe Interaction Potentials", Int. Conf. on the Physics of Electronic and Atomic Collisions, Paris, France, (July 1977).
- 15. I. R. Gatland, L. A. Viehland, and E. A. Mason, "Tests of Alkali Ion-Inert Gas Interaction Potentials by Gaseous Ion Mobility Experiments", Jour. Chem. Phys. 66, 537 (1977).
- 16. M. G. Thackston, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities of Cs<sup>+</sup> Ions in Molecular Gases: H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CO, and CO<sub>2</sub>", Jour. Chem. Phys. 67, 1276 (1977).
- 17. F. L. Eisele, M. G. Thackston, W. M. Pope, I. R. Gatland, H. W. Ellis, and E. W. McDaniel, "Experimental Test of the Generalized Einstein Relation for Cs<sup>+</sup> Ions in Molecular Gases: H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CO, and CO<sub>2</sub>", Jour. Chem. Phys. 67, 1278 (1977).
- 18. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Further Tests of the Generalized Einstein Relation: Cs<sup>†</sup> Ions in Ar, Kr, and Xe", Jour. Chem. Phys. <u>68</u>, 3950 (1978).
- 19. W. M. Pope, H. W. Ellis, F. L. Eisele, M. G. Thackston, E. W. McDaniel, and R. A. Langley, "Mobilities and Longitudinal Diffusion Coefficients for Cs+ Ions in He and Ne Gas", Jour. Chem. Phys. 68, 4761 (1978).
- 20. H. W. Ellis, E. W. McDaniel, D. L. Albritton, L. A. Viehland, S. L. Lin, and E. A. Mason, "Transport Properties of Gaseous Ions Over a Wide Energy Range Part II", Atomic Data and Nuclear Data Tables 22, 179-217 (1978).
- 21. I. R. Gatland, M. G. Thackston, W. M. Pope, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities and Interaction Potentials for Cs<sup>+</sup> Ar, Cs<sup>+</sup> Kr, and Cs<sup>+</sup> Xe", Jour. Chem. Phys. <u>68</u>, 2775 (1978).
- 22. I. R. Gatland, D. R. Lamm, M. G. Thackston, W. M. Pope, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities and Interaction Potentials for Rb+ Ar, Rb+ Kr, and Rb+ Xe", Jour. Chem. Phys. 69, 4951 (1978).
- 23. W. M. Pope, F. L. Eisele, M. G. Thackston, and E. W. McDaniel, "Longitudinal Diffusion Coefficients and Test of the Generalized Einstein Relation for Rb+ Kr, Rb+ Ke, K+ Kr, and K+ Xe", Jour. Chem. Phys. 69, 3874 (1978).
- 24. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, I. R. Gatland, and E. W. McDaniel, "Mobility of Cl Ions in Ne, Ar, and Kr", J. Chem. Phys. 70, 3996 (1979).
- 25. F. L. Eisele, M. G. Thackston, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Longitudinal Diffusion Coefficients and the Generalized Einstein Relation for Cl<sup>-</sup> Ions in Ne, Ar, Kr, and Xe", Jour. Chem. Phys. 70, 5918 (1979).
- 26. S. L. Lin, I. R. Gatland, and E. A. Mason, "Mobility and Diffusion of Protons and Deuterons in Helium a Runaway Effect", J. Phys. B 12, 4179 (1979).

- 27. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Mobilities and Longitudinal Diffusion Coefficients for F- Ions in Kr and Xe", Jour. Chem. Phys. 73, 1477 (1980).
- 28. M. G. Thackston, M. S. Sanchez, G. W. Neeley, W. M. Pope, F. L. Eisele, I. R. Gatland, and E. W. McDaniel, "Mobilities and Longitudinal Diffusion Coefficients for Na<sup>+</sup> Ions in Kr and Xe", Jour. Chem. Phys. 73, 2012 (1980).
- 29. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, E. W. McDaniel, and I. R. Gatland, "Mobility of Cl Ions in Xe Gas and the Cl Xe Interaction Potential", Jour. Chem. Phys. 73, 3183 (1980).
- 30. E. W. McDaniel, "Ionic Transport Phenomena and Their Applications", invited paper presented at Sixth Int. Conf. on Atmospheric Electricity, Manchester, England, July 28 August 1, 1980. Conf. Proceedings to be published (1981).
- 31. H. S. W. Massey, B. Bederson, and E. W. McDaniel (Eds.), Applied Atomic Collision Physics, 4 Vols., Academic, New York, in press.
- 32: D. R. Lamm, M. G. Thackston, F. L. Eisele, H. W. Ellis, J. R. Twist, W. M. Pope, I. R. Gatland, and E. W. McDaniel, "Mobilities and Interaction Potentials for K<sup>+</sup> Ar, K<sup>+</sup> Kr, and K<sup>+</sup> Xe", Jour. Chem. Phys., in press.
- 33. M. G. Thackston, M. S. Sanchez, G. W. Neeley, W. M. Pope, J. R. Twist, and E. W. McDaniel, "The Mobilities and Longitudinal Diffusion Coefficients of Li<sup>+</sup> Ions in Kr and Xe", to be submitted to Jour. Chem. Phys.
- 34. J. R. Twist, F. L. Eisele, M. G. Thackston, F. B. Holleman, R. Chelf, D. R. Lamm, I. R. Gatland, and E. W. McDaniel, "The Mobilities and Longitudinal Diffusion Coefficients of Br Ions in Ne, Ar, Kr, and Xe", to be submitted to Jour. Chem. Phys.
- 35. H. W. Ellis, E. W. McDaniel, and E. A. Mason, "Transport Properties of Gaseous Ions Part III", to be submitted to Atomic Data and Nuclear Data Tables.
- 36. E. W. McDaniel, and E. A. Mason, <u>The Mobility and Diffusion of Ions in Gases</u> (2nd. Ed.), Wiley, New York, in preparation.

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM	7
1. REPORT NUMBER 2. GOVT ACCESSION N	O. 3. HECIPIENT'S CATALOG NUMBER	1
AD- A090	1951	
4. TITLE (and Subtitle)	5. TYPE OF REPORT & PERIOD COVERED	1
	Final	
Pinal Panant	July 1, 1975 - Feb. 28, 1980	
Final Report	6. PERFORMING ORG. REPORT NUMBER	1
7. AUTHOR(*)	8. CONTRACT OR GRANT NUMBER(*)	
E. W. McDaniel and I. R. Gatland	N00014-76-C-0015	1
E. W. MCDaniel and I. R. Gatland	N00014-70-C-0013	
9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS	1
School of Physics	AREA & WORK UNIT NUMBERS	
Georgia Institute of Technology	NR014-314	
Atlanta, Ga. 30332	NK014-314	
11. CONTROLLING OFFICE NAME AND ADDRESS	12. REPORT DATE	1
Office of Naval Research	March 30, 1980	]
Physics Program Office	13. NUMBER OF PAGES	1
Arlington, Va. 22217	6	1
14. MONITORING AGENCY NAME & ADDRESS(If different from Controlling Office)	15. SECURITY CLASS. (of this report)	
	Unclassified	İ
	154. DECLASSIFICATION/DOWNGRADING	ł
•	SCHEDULE	
16. DISTRIBUTION STATEMENT (of this Report)		1
		Į.
Approved for public release; distribution unlimi	ted.	]
approved to prove the provention of the proventi		ļi .
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different	rom Penast)	
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, in uniform	Tom Reports	ļ
		İ
	٠٠,	
18. SUPPLEMENTARY NOTES		
		$\infty$
•	·	
19. KEY WORDS (Continue on reverse side if necessary and identify by block number	10)	
_	•	
Ionic Mobilities Halogen Ions Diffusion Coefficients Noble Gases		
Interaction Potentials		1995
Alkali Ions		0
<b>\</b>	<u> </u>	
20. ABSTRACT (Continue on reverse side if necessary and identify by block number		
The Georgia Tech program of research on ion	ic transport in gases is	C)
described. Experimental measurements of ionic	obilities and diffusion	
coefficients are discussed. The use of the mobile	lity data to obtain ion-	
neutral interaction potentials is described. Re	rerences are given for	
publications covering this report period.		
ľ		<b>\$</b>
ľ		
TOTAL AND		
DD 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE	UNCLASSIFIED	0

